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An overview of the application of Si(Li) detectors to cosmic-ray identification is presented. A vacancy-related defect in FZ silicon that can limit the lithium compensation process in Si(Li) detector fabrication is discussed and a gettering process to remove this defect is outlined. Computer simulation of the gettering process is shown to yield native point defect diffusivity and concentration values approaching those recently proposed by Gösele, Plößl and Tan.[21]

INTRODUCTION

While the consumption of silicon in the fabrication of radiation detectors is an almost insignificant component of the semiconductor industry, the scientific results obtained from silicon radiation detectors over the years have been substantial. Detectors fabricated from large floating-zone (FZ) silicon crystals have been extensively used as sensors for energetic particles and photons in a wide variety of earth-based and space-based experiments. Space applications include:

- studies of the elemental, isotopic, and charge state composition of energetic particles accelerated in the galaxy, on the sun and in the interplanetary medium.
- spectroscopic studies of astrophysical x-ray emitters.
- calorimetric measurements of the energies of relativistic electrons and positrons in the cosmic rays.

Driven by the need to fabricate increasingly larger devices, detector development has also made significant contributions to the characterization of impurities and defects in semiconductors. These include:

- identification of deep levels in the semiconductor bandgap via Deep Level Transient Spectroscopy.

nucleosynthesis processes were involved in the formation of our solar system and the galaxies beyond.

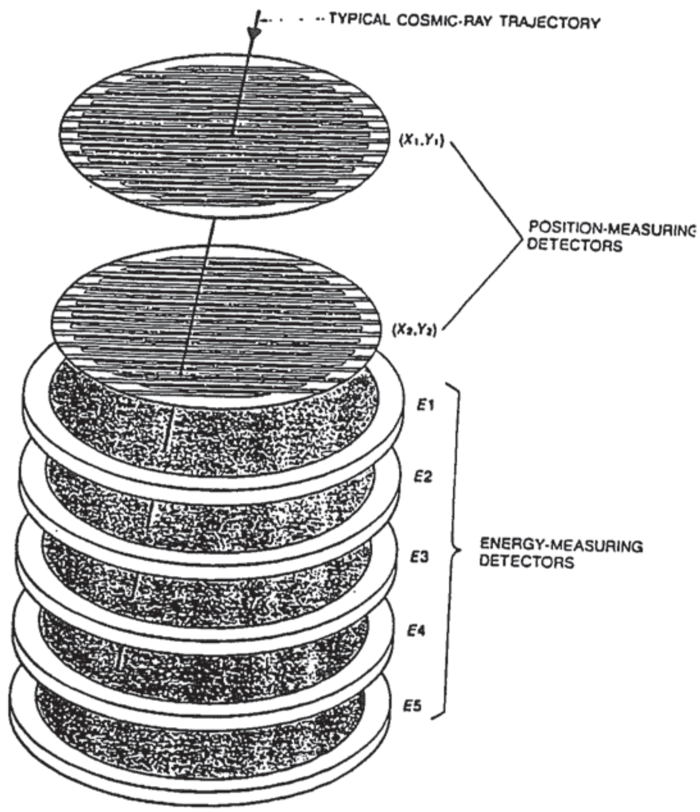

Fig. 1. Typical arrangement of a Si(Li) detector based cosmic-ray telescope. To improve the resolving power of the cosmic ray telescope, the trajectory of the incident cosmic ray is determined by the position sensitive detectors (X_1Y_1 and X_2Y_2). The energy loss for each cosmic ray detected by the telescope is then adjusted, based upon the trajectory information, to an equivalent normal angle of incidence.[3]

TELESCOPE SILICON DETECTORS

Over the past twenty-five years silicon detector based cosmic-ray telescopes have been designed to identify galactic cosmic rays ranging in energy from 10 - 10^4 MeV/u.[2] To detect these energetic particles, stacks of relatively thick silicon detectors (3 - 5 mm), as shown in Fig. 1, are normally employed. For example, the CRIS telescope, which is designed to detect cosmic rays ranging in energy from 50 to 500 MeV/u, and in atomic

LITHIUM DRIFTED SILICON DETECTORS

One of the results from semiconductor research conducted in the early 1960's was that interstitial lithium ion donors would pair with or compensate acceptor ions in silicon and germanium crystals resulting in regions with very small net-impurity concentrations.[6] This result has been used in the intervening years by various laboratories and commercial companies to produce Si(Li) radiation detectors. The compensation process (or "drifting") is illustrated schematically in Fig. 4. In *p*-type silicon, the lithium-ion pairing occurs so completely with the boron acceptors present that a region is formed which is almost free of any electrically active impurity centers. The net-impurity concentration can approach $1 \times 10^9/\mathrm{cm}^3$, which is about two orders of magnitude lower than can be reached by current high-purity silicon crystal growing techniques. This low net-impurity concentration permits *p*-Si wafers several mm thick to be fully depleted with relatively modest bias voltages applied across the *p-i-n* junction.

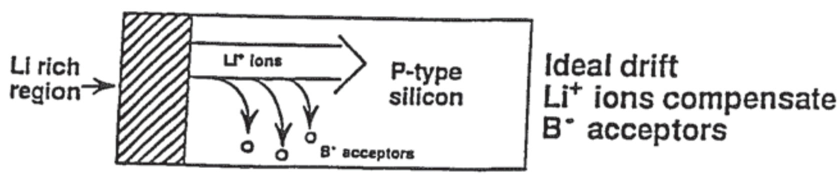

Fig. 4. A schematic representation of the lithium-ion compensation process. The interstitial positive lithium ions drift in an electric field produced by an external bias from the Li- doped region to the acceptor doped *p*-type region compensating any acceptors encountered and forming an intrinsic region.

Figure 5 further illustrates this lithium-ion compensation process. Si(Li) detector fabrication begins by diffusing (375 °C , 15 minutes) lithium into a *p*-type silicon wafer to form a n^+-p junction with the resulting lithium diffusion profile approximated by the dotted line(**1**) in the figure. By heating the wafer to ~ 110 °C and applying a reverse bias across the n^+-p junction, the positive lithium donor ions are forced by the applied electric field from the n^+ lithium region into the *p*-type bulk region, compensating or pairing with the acceptors. After some time, the lithium-ion profile assumes the shape represented by the solid line(**2**) in the figure, at which point the following differential equation describes the growth rate of the lithium-ion compensated region:

$$N_A\, dW/dt = \mu_L N_A E - N_L W R_L, \text{ or}$$

$$= \mu_L N_A V/W - N_L W R_L, \qquad [1]$$

Silicon crystals often have imperfections that can act as lithium-ion "loss" sites. These sites, as can be seen from Eq. 2, become more dominant in higher resistivity (low N_A) silicon.

Within these two resistivity bounds, experience in fabricating Si(Li) detectors at the Lawrence Berkeley National Laboratory (LBNL), over many years, indicates that *p*-type floating-zone (FZ) crystals with the specifications given in Table I normally result in Si(Li) detectors that are completely compensated.

Table I: *p*-Type FZ Silicon Specifications for Si(Li) Detector Fabrication

Parameter	Value
Resistivity (Ohm-cm)	1,000-2,000
Lifetime (μs)	>1,000
Orientation	< 1 1 1 >
Oxygen (cm^{-3})	$< 10^{16}$

However, in recent years we often have encountered FZ silicon crystals with these nominal specifications that still cannot be successfully lithium-ion compensated. A potential difficulty with the compensation process is apparent in the solution to Eq. 2. Assuming that V, μ_L, and R_L remain constant, the compensated region width, $W(t)$, after a drift time, t, is:

$$W(t) = W_{max} \left(1 - e^{-2t/\tau} \right)^{1/2} \qquad [3]$$

where $t > 0$, $W_{max} = (\mu_L V \tau)^{1/2}$, and $\tau = N_A/(N_L R_L)$ is the effective Li^+ ion lifetime. If the lithium-ion loss is significant, then $\tau << t$ may exist. Equation 3 then predicts that the maximum compensated depth can only approach W_{max}, independent of the drift time.

FABRICATION OF SI(LI) DETECTORS

As noted above, fabrication of Si(Li) detectors is a low temperature process. An abbreviated LBNL process sequence for fabricating Si(Li) detectors is shown in Fig. 6. We have discussed this process sequence in detail earlier and mainly show here the thermal budget involved.[7]

crystal diameter where one defect type dominates over all the others.[13] Their results are shown schematically in Fig. 8. Their observation, that the center of FZ crystals can have a high concentration of D defects, is strikingly similar to our conclusion that the difficulty in lithium compensating the center of some FZ silicon crystals, as shown in Fig. 7, is caused by the presence of vacancy-related defects.

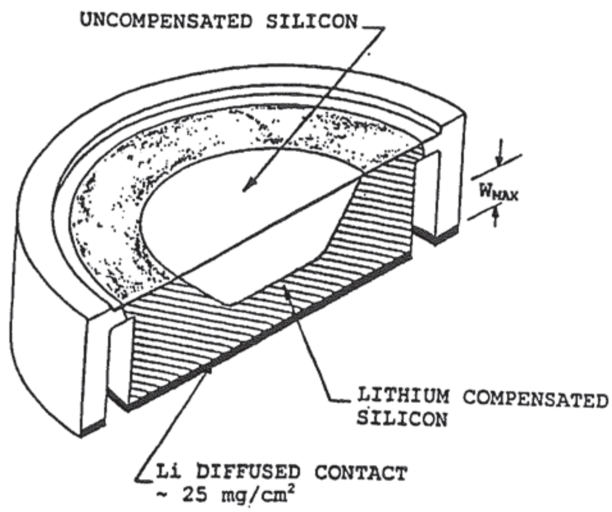

Fig. 7. A sketch of a ~40 mm diameter, 5 mm thick Si(Li) detector fabricated on a 50 mm diameter FZ *p*-type wafer. The lithium-ion compensated region was decorated on the actual device by copper staining, which is essentially a room temperature copper-silicon displacement reaction.[9]

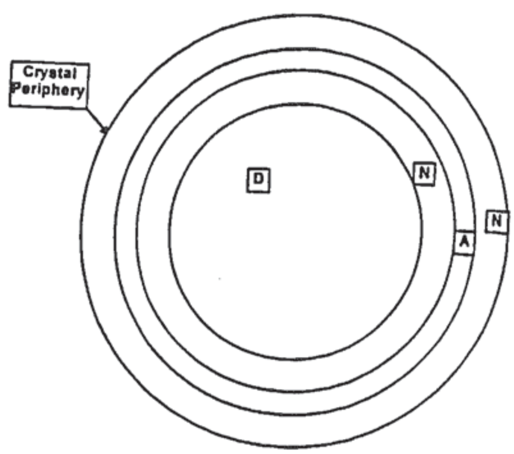

Fig. 8. A sketch showing the concentric regions in a FZ Si crystal in which different point defects dominate.[13] The regions containing D defects, A Defects and no defects are denoted by the letters **D**, **A**, and **N**, respectively.

The diffusivity, concentration, and bulk recombination constants are given by:

$$D_{I,V} = D_o^{I,V} \exp\left(-E_D^{I,V}/k_B T\right) \text{ cm}^2/\text{s} \tag{8}$$

$$C_{I,V}^{*} = C_o^{I,V} \exp\left(-E_C^{I,V}/k_B T\right) \text{ cm}^{-3} \tag{9}$$

$$K_r^{I,V} = K_o^{I,V} \exp\left(-E_K^{I,V}/k_B T\right) \text{ cm}^3/\text{s} \tag{10}$$

where the pre-exponential factors and the enthalpy (E) terms are commonly referred to as point defect parameters determined by fitting, as discussed in the next section.

Recently, the influence of high substitional carbon concentrations on the silicon native point defect diffusivities has been studied by the Poate group at AT&T.[20] Based on these results, Gösele, Plößl and Tan in a recent review suggested that many of the experimental values obtained for the native point defect diffusivities and concentrations may have been influenced by the presence of carbon in the crystals.[21] They proposed that the theoretical values derived by Konoplev and Heinig[22] should be taken as bounds on these parameters and provided plots of these estimates, which are replicated in Fig. 9.

SUPREM-IV MODELING

A flexible solution routine to Eqns. 6-7 is contained in the process modeling program SUPREM-IV[23] and we have used this program to model our gettering process on 3 mm thick wafers. To simulate the reduction of vacancies over a depth of ~1.5 mm, as shown in Fig. 10, we have had to adjust the SUPREM-IV program default coefficients for the native point defect concentrations and diffusivities. Our latest values for these parameters are:

$$D_I = 1\,x10^3 \; exp\,(-2.44\; eV/kT)\; cm^2/sec \tag{11}$$

$$C_I = 2.5\,x10^{19} \; exp\,(-2.36\; eV/kT)\; cm^{-3} \tag{12}$$

$$D_V = 1\,x10^2 \; exp\,(-2.92\; eV/kT)\; cm^2/sec \tag{13}$$

$$C_V = 5\,x10^{13} \; exp\,(-1.08\; eV/kT)\; cm^{-3}, \tag{14}$$

which we expect to adjust further upon completion of planned experiments and subsequent analyses. Equations 11-14 are plotted in Fig. 9 along with the limiting values proposed by Gösele, Plößl, and Tan.[21]

collecting area telescopes such as that mentioned earlier in the CRIS telescope design (4 detector stacks, each stack ~70 cm^2 in area). In such telescope designs larger diameter detectors are advantageous. For example, if FZ Si crystals 125 mm in diameter had been available, then only 3 detector stacks would have been required to achieve the same collecting power as the CRIS telescope, reducing the instrument's complexity and power consumption, both of which are of crucial importance in space-based instruments.

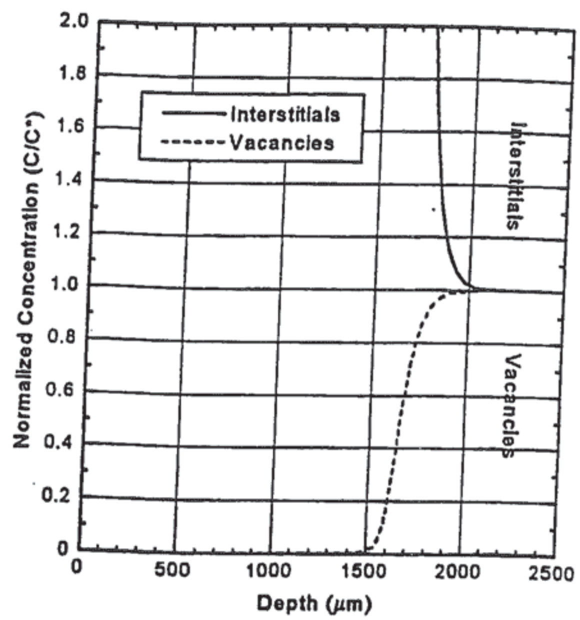

Fig. 10. The SUPREM-IV[23] computer program simulation of the normalized vacancy and silicon interstitial concentrations for a 100 minute, 950 °C gettering process. The SUPREM-IV program default diffusivity and concentration coefficients were adjusted to produce a ~1.5 mm wide region in which the vacancy concentration is significantly reduced. The coefficients used here are given in Eqs. 11-14.

Both our gettering experiments and computer simulations to date suggest that we can reduce or remove the vacancy-like defects from the center of FZ crystals by gettering. And while we can make usable Si(Li) detectors on the gettered wafers[24], the 950 °C process temperature raises the risk of contaminating the wafers with unwanted deep level impurities (e.g., Fe, Cu and Au) that can degrade Si(Li) detector performance. Since we have obtained 100 mm diameter crystals that apparently have sufficiently low D defect concentrations for our Si(Li) process[25], there are FZ growth conditions that minimize or avoid the growth of D defects in the center of the crystals. These growth conditions have been well demonstrated on smaller diameter crystals.[12] Therefore, rather than gettering

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